TITLE: Singlet and Triplet States of X+ and X- Trions in a 2D Quantum Well

9th Int. Symp. "Nanostructures: Physics and Technology"
St Petersburg, Russia, June 18–22, 2001

Singlet and triplet states of X^+ and X^- trions in a 2D quantum well

R. A. Sergeev and R. A. Suris
Ioffe Physico-Technical Institute, St Petersburg, Russia

Abstract. A new simple variational wave function with a few variational parameters for 2D X^+ and X^- trions has been suggested. The function gives accurate results for the singlet and triplet state energies of X^+ and X^- trions in the whole range of electron-to-hole mass ratio. The mass ratio range where the triplet state exists has been found, and the behavior of the triplet state energy has been examined near the critical mass ratio.

Introduction

Three particle electron-hole complexes (trions) in bulk semiconductors were considered by Lampert in 1958 [1]. A trion is an analog of the ion H^- that was firstly considered by Bethe [2]. However, the experimental investigation of trions in bulk semiconductors is made difficult by their small binding energy.

Recently interest in experiment and theory of trions has quickened due to considerable progress in heterostructure synthesis. The theoretical calculations performed in the 1980s [3–6] predicted a substantial (up to tenfold) increase of trion binding energy in quantum well heterostructures as against bulk trions. This made possible experimental studies which were firstly performed by K. Kheng et al. [7].

In recent years the trion energies versus the effective mass ratio were intensively studied in a two-dimensional case or in a single quantum well [8–14]. Nevertheless, only a singlet state of trions in a zero magnetic field was considered. In 1958 Lampert [1] predicted the existence of triplet state for the complex consisting of two heavy carriers (holes) and one light particle (electron) for a large hole-to-electron mass ratio when the trion is an analog of molecule H_2^+. He pointed out that it would be of interest to fix the mass ratio region where the complex exists. However, the triplet state of trion in a zero magnetic field is not completely studied up to now. Some calculations of trion triplet state were performed only for the 3D case [15–17].

In this paper we consider singlet and triplet states of 2D trion in the whole range of mass ratio. Using simple variational calculations, we find the mass ratio region where the triplet trion exists.

1. Singlet state

For singlet state variational calculations, the following symmetric coordinate trial function was used:

$$\psi_s(\vec{r}_1, \vec{r}_2) = (\exp(-ar_1 - br_2) + \exp(-ar_2 - br_1))\frac{1 + cR}{1 + d(R - R_0)^2}\exp(-sR), \quad (1)$$

where $\vec{r}_1$ and $\vec{r}_2$ are the 2D vectors from hole (for simplicity the terms of X^- are used) to electrons, $R = |\vec{r}_1 - \vec{r}_2|$ is the distance between two electrons, a, b, c, d, R_0, and s are the variational parameters. The parameters a and b are the reciprocal radii of two electron

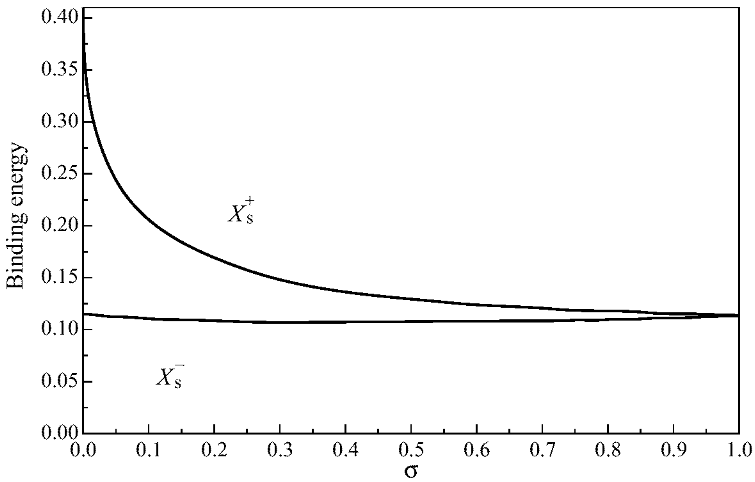

Fig. 1. Singlet state binding energies of 2D X^- and X^+ trions versus $\sigma = m_e^*/m_h^*$. The energy is measured in 2D exciton binding energy units.

orbits. The parameter c corresponds to the polarization of electron-hole pair by the third charged particle. The parameter d takes into account longitudinal oscillations of two equal particles near the equilibrium distance R_0. These two parameters are essentially important for the calculation of trion energy in the mass ratio region near the molecule H_2^+-like trion. The parameter s is used to correct the trion wave function at large distances. Reasonable results can be obtained even without the use of the latter parameter. A detailed discussion of the variational function is presented in [18].

The singlet state energy versus the electron-to-hole mass ratio, $\sigma = m_e^*/m_h^*$, is shown in Fig. 1. It should be noted that as expected, the energy behaves as square root of σ at $\sigma \to 0$.

We would like to stress that we obtained the binding energy dependence for whole domain of the electron-to-hole mass ratio (Fig. 1) using the same trial wavefunction with only 6 parameters. Actually, the limit $\sigma \to 0$ is difficult for consideration due to delta-like shape of the wavefunction on $R - R_0$ for two heavy particles. It is why the calculations in [5] were limited with $\sigma > 0.1$. A sophisticated variational technique for the charge exciton energy calculations was developed in [13]. The technique gives very precise results in the whole mass ratio domain. However, in contrast to our rather simple calculations, the trial wavefunction shape in [13] depends on the mass ratio and the number of variational parameters increases with decrease of the mass ratio.

In spite of a rather small number of the variational parameters used, our results are in good agreement with results of more sophisticated calculations [5, 8, 10, 13].

2. Triplet state

We take the triplet state trial function as an antisymmetrized singlet state function (1):

$$\psi_t(\vec{r}_1, \vec{r}_2) = \left[\exp(-ar_1 - br_2) + \exp(-ar_2 - br_1)\right] \frac{R\exp(-sR)}{1 + d(R - R_0)^2} \exp(i\theta_R), \quad (2)$$

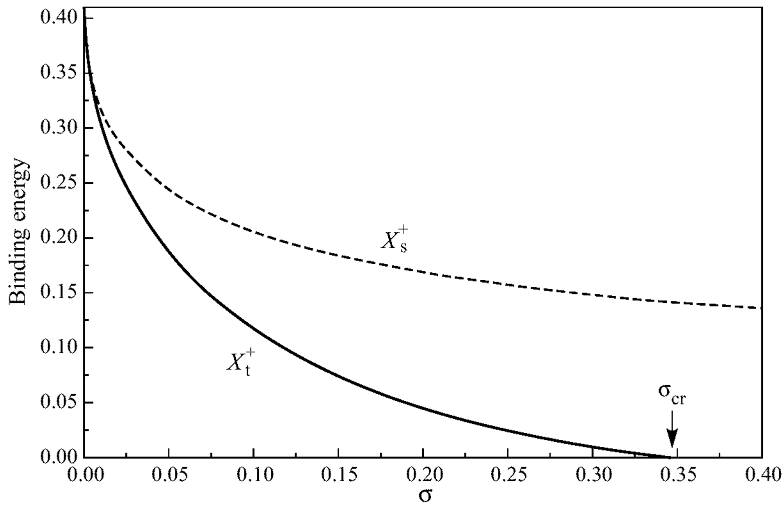

Fig. 2. The binding energy of 2D triplet X^+ trion (solid) versus $\sigma = m_e^*/m_h^*$ (in 2D exciton binding energies). The dashed curve is the singlet state X^+ binding energy.

where θ_R is the angle between the vector $\vec{R}$ and a certain direction given beforehand. The factor $\exp(i\theta_R)$ describes the antisymmetry of triplet state wave function and corresponds to the whole trion momentum $l = 1$.

Figure 2 shows the triplet state binding energy of X^+ trion versus the mass ratio. For reference, the singlet energy dependence is also plotted.

As was found from variational calculations, the triplet state vanishes, transforming into a resonant state at the critical mass ratio $\sigma_{cr} \approx 0.35$. The variational method gives the energy value that cannot be lower than its exact value. Therefore, the critical value of mass ratio provided by this method cannot exceed its exact value.

Let the triplet state binding energy of trion versus $\sigma - \sigma_{cr}$ be found near the critical value of mass ratio. We notice that this problem is analogous to the problem on vanishing the bound state of a particle with the momentum $l = 1$ in a 2D potential. In this case we have

$$E\ ln\left(\frac{E_{eff}}{E}\right) = -A(\sigma - \sigma_{cr}), \tag{3}$$

where E is the binding energy of trion triplet state in relation to the decomposition to an exciton and a free particle. The positive parameters E_{eff} and A can be evaluated from the variational calculations:

$$E_{eff} \approx 2.70; \qquad A \approx 1.17. \tag{4}$$

3. Conclusion

Simple variational wave functions with a few variational parameters are suggested to calculate with a good accuracy the singlet and triplet state energies of 2D X^+ and X^- trions in the whole range of electron-to-hole effective mass ratio. In a zero magnetic field, the trion triplet state is found to exist in a considerable mass ratio area close to the H_2^+-like trion. The critical value of electron-to-hole mass ratio is found to be more than 0.35.

Acknowledgments

This work was supported by the Russian Foundation for Basic Research, Grants 99-02-16796, 00-02-04020NNIO_a, and by the Federal Program on Support of Leading Scientific Schools, Grant 00-15-96812.

References

[1] M. A. Lampert, *Phys. Rev. Lett.* **1**, 12, 450 (1958).
[2] H. A. Bethe, *Z. Phys.* **57**, 815 (1929).
[3] B. Stebe and C. Comte, *Phys. Rev. B* **15**, 8, 3967 (1977).
[4] R. Schilling and D. C. Mattis, *Phys. Rev. Lett.* **49**, 11, 808 (1982).
[5] B. Stebe and A. Ainane, *Superlatt. Microstruct.* **5**, 4, 545 (1989).
[6] Z. Chen and C. D. Lin, *Phys. Rev. A* **42**, 1, 18 (1990).
[7] K. Kheng, R. T. Cox, Y. M. d'Aubigne, F. Bassani, K. Saminadayar and S. Tatarenko, *Phys. Rev. Lett.* **71**, 11, 1752 (1993).
[8] A. Thilagam, *Phys. Rev. B* **55**, 12, 7804 (1996).
[9] B. Stebe, G. Munschy, L. Stauffer, F. Dujardin and J. Murat, *Phys. Rev. B* **56**, 19, 12454 (1997).
[10] J. Usukura, Y. Suzuki and K. Varga *Phys. Rev. B* **59**, 9, 5652 (1999).
[11] W. Y. Ruan, K. S. Chan, H. P. Ho, R. Q. Zhang and E. Y. B. Pun, *Phys. Rev. B* **60**, 8, 5714 (1999).
[12] B. Stebe, A. Moradi and F. Dujardin, *Phys. Rev. B* **61**, 11, 7231 (2000).
[13] A. Esser, E. Runge and R. Zimmermann *Phys. Rev. B* **62**, 12, 8232 (2000).
[14] C. Riva, F. M. Peeters, K. Varga, *Phys. Status Solidi A* **178**, 1, 513 (2000).
[15] A. P. Mills, Jr. *Rhys. Rev. A* **24**, 6, 3242 (1981).
[16] A. K. Bhatia, R. J. Drachman, *Rhys. Rev. A* **28**, 4, 2523 (1983).
[17] A. K. Bhatia and R. J. Drachman, *Rhys. Rev. A* **35**, 10, 4051 (1987).
[18] R. A. Sergeev and R. A. Suris, to be published in *Phys. Solid State* **43**, 4 (2001), [translated from *Fiz. Tverd. Tela* **43**, 4, 714 (2001)].